

Acta Crystallographica Section D

Volume 70 (2014)

Supporting information for article:

Structure solution of DNA binding proteins and complexes with
ARCIMBOLDO libraries

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Table S1 Zinc-finger type.

PDB	Description	Res. [Å]	R/R _{free} [%]	Reference	rmsd/No of C α *	No of C α **	No. in Fig. 3 (Chain)
1A1G	Zif268- DNA	1.9	0.215/0.27	(Elrod-Erickson <i>et al.</i> , 1998)	0.8/30	30	1
1A1H	Zif268- DNA	1.6	0.235/0.277	(Elrod-Erickson <i>et al.</i> , 1998)	0.6/30	30	2
1A1I	Zif268- DNA	1.6	0.191/0.216	(Elrod-Erickson <i>et al.</i> , 1998)	0.6/29	29	3
1A1J	Zif268- DNA	2.0	0.210/0.262	(Elrod-Erickson <i>et al.</i> , 1998)	0.5/30	30	4
1A1K	Zif268- DNA	1.90	0.210/0.259	(Elrod-Erickson <i>et al.</i> , 1998)	0.6/30	30	5
1A1L	Zif268- DNA	2.30	0.196/0.267	(Elrod-Erickson <i>et al.</i> , 1998)	0.6/30	30	6
1AAY	Zif268- DNA	1.60	0.195/0.242	(Elrod-Erickson <i>et al.</i> , 1998)	0.5/30	30	7
1F2I	Zinc-finger- DNA	2.35	0.215/0.256	(Wang <i>et al.</i> , 2001)	0.5/31	31	8 (G) 9 (H) 10 (K)
1G2D	Zinc-finger- DNA	2.20	0.225/0.262	(Wolfe <i>et al.</i> , 2001)	0.6/31	31	11 (C) 12 (F)
1G2F	Cys2His2 Zinc-finger	2.00	0.233/0.263	(Wolfe <i>et al.</i> , 2001)	0.6/31	31	13 (C)
1JK1	Zif-268- DNA	1.90	0.214/0.266	(Miller & Pabo, 2001)	0.5/30	30	14
1JK2	Zif268- DNA	1.65	0.230/0.273	(Miller & Pabo, 2001)	0.7/30	30	15 (A)
1LLM	Zif23- GCN4-DNA	1.5	0.216/0.234	(Wolfe <i>et al.</i> , 2003)	0.7/29	29	16 (C) 17 (D)
1MEY	Zinc-finger- DNA	2.2	0.224/0.319	(Kim & Berg, 1996)	0.7/29	29	18 (C) 19 (F)
1P47	Tandem-Zif- DNA	2.2	0.219/0.267	(Peisach & Pabo, 2003)	0.6/30	30	20 (B) 21 (A)

1TF6	TFIIIA-Zif- DNA	3.1	0.308/0.363	(Nolte <i>et al.</i> , 1998)	0.9/31	31	22
1UBD	YY1-DNA	2.50	0.212/0.33	(Houbaviy <i>et al.</i> , 1996)	0.7/31	31	23
1UN6	Zinc-finger- RNA	3.1	0.216/0.259	(Lu <i>et al.</i> , 2003)	1.4/31	30	24 (B) 25 (C) 26 (D)
1ZAA	Zif268- DNA	2.1	0.182/n.a.	(Pavletich & Pabo, 1991)	0.6/30	30	27
2DRP	Zinc-finger- DNA	2.80	0.193/n.a.	(Fairall <i>et al.</i> , 1993)	1.7/29	27	28 (A) 29 (D)
2GLI	Five-finger- DNA	2.60	0.228/n.a.	(Pavletich & Pabo, 1993)	0.7/31	31	30
2HGH	TFIII Zinc- finger	NMR	NMR	(Lee <i>et al.</i> , 2006)	1.2/31	31	31
2I13	Aart-DNA	1.96	0.203/0.249	(Segal <i>et al.</i> , 2006)	0.6/29	29	32 (B) 33 (A)
2J7J	Zinc-finger- DNA	1.65	0.218/0.228	(Lu & Klug, 2007)	1.7/31	30	34
2JP9	Wilms- Tumor Zinc- finger-DNA	NMR	NMR	(Stoll <i>et al.</i> , 2007)	0.7/29	29	35
2JPA	Wilms Factor Zinc- finger	NMR	NMR	(Stoll <i>et al.</i> , 2007)	1.5/31	30	36
2KMK	Gfi-1 Zinc- finger-DNA	NMR	NMR	(Lee <i>et al.</i> , 2010)	0.8/29	30	37
2PRT	Wilms- Tumor Zinc- finger-DNA	3.15	0.236/0.277	(Stoll <i>et al.</i> , 2007)	0.5/31	31	38
2WBU	KLF4-DNA	2.5	0.220/0.278	(Schuetz <i>et al.</i> , 2011)	0.4/31	31	39
3IUF	C2H2 Zinc- finger	1.8	0.195/0.237	(Zhang <i>et al.</i> , 2011)	1.6/28	26	40
3MJH	C2H2 Zinc- finger	2.0	0.196/0.260	(Mishra <i>et al.</i> , 2010)	1.5/27	27	41 (B) 42 (D)

* number of equivalent C α -atoms used by DALI.

** number of C α -atoms in the pdb files used for ARCIMBOLDO trials.

Table S2 Zipper-type.

PDB	Description	Res. [Å]	R/R _{free} [%]	reference	No of C α **
1GTW	C/EPB beta-DNA	1.85	0.231/0.271	PDB	30+29
1H8A	c-Myb/EPB beta-DNA	2.23	0.245/0.288	(Tahirov <i>et al.</i> , 2002)	30+30
1JNM	Jun/Cre-DNA	2.20	0.228/0.286	PDB	30+30
2C9L	Zipper-DNA	2.25	0.232/0.264	(Petosa <i>et al.</i> , 2006)	30+30
2H7H	Jun BZIP-DNA	2.3	0.224/0.274	PDB	30+30

** number of C α -atoms in the pdb files used for ARCIMBOLDO trials.

Table S3 Three-helix bundle HTH.

PDB	Description	Res. [Å]	R/R _{free} [%]	reference	rmsd/No of C α *	No of C α **
1i6x	Star mutant CRP	2.2	0.230/0.2691	PDB	0.48/14	54
1lj9	SlyA	1.60	0.248/0.275	(Wu <i>et al.</i> , 2003)	1.05/23	41
1rp3	sigma/anti sigma complex	2.3	0.242/0.262	(Sorenson <i>et al.</i> , 2004)	3.21/23	46
1sfx	transcriptional regulator	1.55	0.150/0.183	PDB	3.21/23	41
1tqm	Rio2	1.99	0.174/0.228	(LaRonde-LeBlanc & Wlodawer, 2004)	0.97/26	46
1zar	Rio2 with ADP	1.75	0.185/0.218	(LaRonde-LeBlanc <i>et al.</i> , 2005)	0.98/26	46
1zyr	Tt RNA polymerase	3.0	0.261/0.282	(Tuske <i>et al.</i> , 2005)		44
2hr3	PA transcriptional regulator	2.4	0.212/0.280	PDB	1.16/26	42
2hyf	BS MntR	2.80	0.217/0.277	(DeWitt <i>et al.</i> , 2007)	1.20/26	45
2it0	Ider-DNA	2.60	0.229/0.273	(Wisedchaisri <i>et al.</i> , 2007)	1.07/26	45
2ivm	Mtb regulatory protein	2.5	0.201/0.255	(Shrivastava & Ramachandran, 2007)	0.72/26	41
2p6t	NG regulator	2.9	0.239/0.300	(Ren <i>et al.</i> , 2007)	1.03/26	40

2zny	FFRP	2.59	0.54/0.258	(Yamada <i>et al.</i> , 2009)	0.69/26	41
3cta	Riboflavin kinase	2.20	0.237/0.270	PDB	0.98/26	47
3eco	MepR	2.40	0.242/0.289	(Kumaraswami <i>et al.</i> , 2009)	1.17/26	43
3f22	Zalpha-DNA	2.50	0.224/0.269	(Ha <i>et al.</i> , 2009)	0.93/26	44
3hrt	ScaR	2.80	0.230/0.282	(Stoll <i>et al.</i> , 2009)	1.05/26	45
3jsp	LexA-DNA	2.90	0.267/0.287	(Zhang <i>et al.</i> , 2010)	2.65/27	47
3ngo	CNOT6L nuclease	2.20	0.217/0.263§	PDB	0.89/26	43
2q5f	LMNASK1	1.90	0.189/0.222	(Poncet-Montange <i>et al.</i> , 2007)	1.1/26	42

* number of equivalent C α -atoms used by DALI.

** number of C α -atoms in the pdb files used for ARCIMBOLDO trials.

Table S4 Helix-turn-helix motif plus DNA-fragment

PDB	Description	Res [Å]	R	reference	rmsd*
1akh	MAT α 1/MAT α 2-DNA	2.50	0.201/0.302	(Li <i>et al.</i> , 1998)	0.43
1au7	Pit-1/DNA	2.30	0.230/0.302	(Jacobson <i>et al.</i> , 1997)	0.73
1b8i	UBX/EXD-DNA	2.40	0.224/0.304	(Passner <i>et al.</i> , 1999)	0.36
1du0	Homeodomain DNA	2.00	0.237/0.270	(Grant <i>et al.</i> , 2000)	0.59
1fjl	Drosophila homeodomain-DNA	2.0	0.198/na	(Wilson <i>et al.</i> , 1995)	0.39
1gt0	POU/HMG/DNA	2.60	0.232/0.285	(Reményi <i>et al.</i> , 2003)	0.53
1yrn	MAT α 1/MAT α 2-DNA	2.50	0.225/0.298	(Li <i>et al.</i> , 1995)	0.41
2d5v	HNF6 α -DNA	2.00	0.247/0.269	(Iyaguchi <i>et al.</i> , 2007)	0.63
2h1k	Pdsx homeodomain DNA	2.42	0.227/0.277	(Longo <i>et al.</i> , 2007)	0.60
2hdd	Engrailed homeodomain DNA	1.90	0.205/0.251	(Tucker-Kellogg <i>et al.</i> , 1997)	0.52
2r5z	Hox-DNA	2.60	0.233/0.303	(Joshi <i>et al.</i> , 2007)	0.39
9ant	Antennapeida- homeodomain DNA	2.40	0.218/0.239	(Fraenkel & Pabo, 1998)	0.41

* root-mean-square deviation of 31 equivalent C-alpha atoms treated as one rigid block compared to the correct solution of 3RKQ.

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